Recent Developments in FUN3D: Entropy Stable DG-FEM

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http://fun3d.larc.nasa.gov

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- Bill Jones, NASA Langley Research Center
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  - Previously Purdue Univ PhD student in residence at NASA Langley Research Center

Motivation

Overview

CFD Vision 2030 Study: A Path to Revolutionary Computational Aero

NASA/CR-2014-218178: Slotnick, Khodadoust, Alonso, Darmofal, Gropp, Lurie, and Mavriplis

Summary

- Applications
  - “Complex flows with BL transition and smooth body separation”
  - Off-design unsteady simulations (stall prediction)
  - LES and Hybrid RANS-LES models
  - Subsonic, transonic, supersonic
- Next generation numerical algorithms
  - High-order (HO) methods**
  - Low dissipation / dispersion
  - Foundational approaches (high risk / high payoff research)
- Robust automation
  - Routine hands-off convergence in all circumstances
  - Novel robust numerical techniques
    - Entropy-preserving schemes offer possibilities of radical advances

** HO spatial operators are well suited for time-dependent simulations. Error accumulates (spatial, temporal, algebraic).

Vision Statement

A brief history of HO methods

- Kreiss-Oliger, 1972; Gottlieb-Orszag, 1977
- Brisk development in 80’s; Canuto-Hussaini-Quarteroni-Zang, 1987

What happened? Instability happened!

- Informal poll of practitioners: Fragile in real world applications
- ICOSAHOM 2014 (Int. Conf. Spectral & High-Order Methods)
  - 200 papers: 20% mentioned “stability” in title
  - Stab(le)(ility)(ilize) (27 papers)
  - Filter/alias/dissipation (12 papers)
- Move from experimentation to mathematics!

Vision 2019 (August 18)

The nonlinear equations are stable in nature,
as should be their discrete representation.

- Maturation of nonlinear stability theory: Turning the corner
- Growing body of schemes with nonlinear stability proofs

Statement: Achieve robustness of current 2nd-order FV schemes

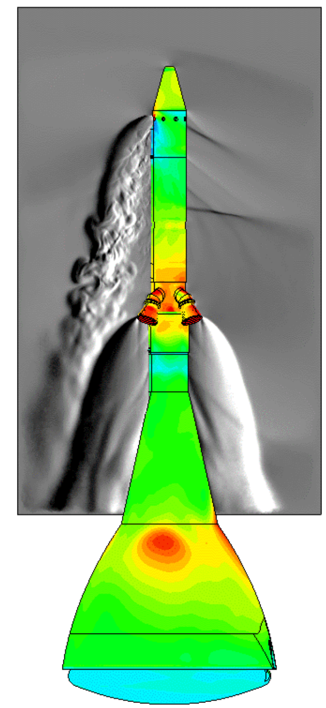
What's the Plan?

Entropy Stable Spectral Collocation (plus BCs)

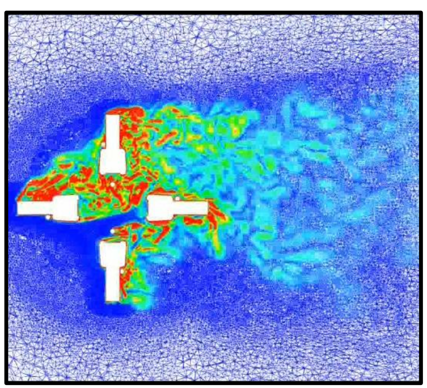
- Three pillars: Stability, accuracy, conservation
- Conservation form operator: Mass, momentum, energy
  - Secondary invariant: Entropy
- Applicable for capturing shocks (Rankine-Hugoniot via Lax-Wendroff Thm)

Implement in FUN3D

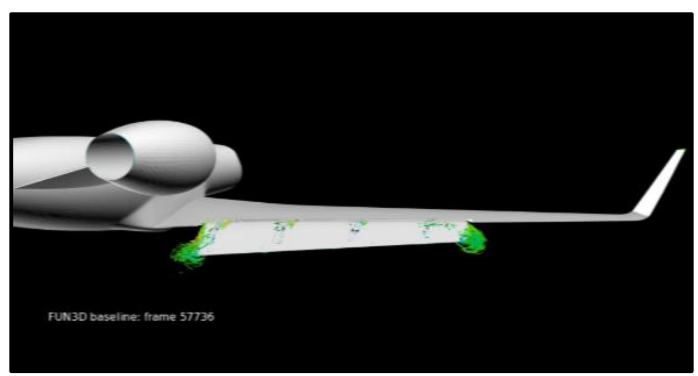
- Established infrastructure and customer base
- Increasing need for HO capability
  - DNS / LES / DES / URANS
  - Aeroacoustics, electromagnetics
  - Rotorcraft
  - Separated flows, stall
  - Mixing



Orion Launch Abort System



Rotor Hub Courtesy Georgia Tech



G550 Courtesy NASA / Gulfstream Partnership for Airframe Noise Research

Entropy Stability

Compressible Navier-Stokes Equations

$$q_t + \left(f_i^{(I)}\right)_{x_i} = \left(f_i^{(V)}\right)_{x_i}, \quad x \in \Omega, \quad t \in [0, \infty),$$

$$q|_{\partial\Omega} = g^{(B)}(x,t), \quad x \in \partial\Omega, \quad q(x,0) = g^{(0)}(x), \quad x \in \Omega$$

Entropy variables: S_q with $S = -\rho s$

Entropy fluxes: $F_i = -\rho u_i s$

Entropy equation:

$$S_q q_t + S_q \left(f_i^{(I)}\right)_{x_i} = S_t + (F_i)_{x_i} = S_q \left(f_i^{(V)}\right)_{x_i} = \left(w^\top f_i^{(V)}\right)_{x_i} - w_{x_i}^\top \widehat{c}_{ij}\, w_{x_j}$$

Global conservation statement:

$$\frac{d}{dt}\int_\Omega S \,\mathrm{d}\mathbf{x} = \left[w^\top f_i^{(V)} - F_i\right]_{\partial\Omega} - \int_\Omega w_{x_i}^\top \widehat{c}_{ij}\, w_{x_j} \,\mathrm{d}\mathbf{x}$$

Semi-Discrete Form

$$S_q q_t + S_q \left(f_i^{(I)}\right)_{x_i} = S_t + (F_i)_{x_i} = S_q \left(f_i^{(V)}\right)_{x_i} = \left(w^\top f_i^{(V)}\right)_{x_i} - w_{x_i}^\top \widehat{c}_{ij}\, w_{x_j}$$

Summation-by-Parts telescoping form:

$$\mathbf{q}_t = \mathcal{P}_{x_i}^{-1} \Delta_{x_i} \left(-\overline{\mathbf{f}}_i^{(I)} + \overline{\mathbf{f}}_i^{(V)}\right) + \mathcal{P}_{x_i}^{-1}(\mathbf{g}^{(B)} + \mathbf{g}^{(In)})$$
$$\mathbf{q}(x,0) = \mathbf{g}^{(0)}(x), \quad x \in \Omega$$

- $\mathbf{g}^{(B)}$ contains BC data
- $\mathbf{g}^{(In)}$ interface penalty

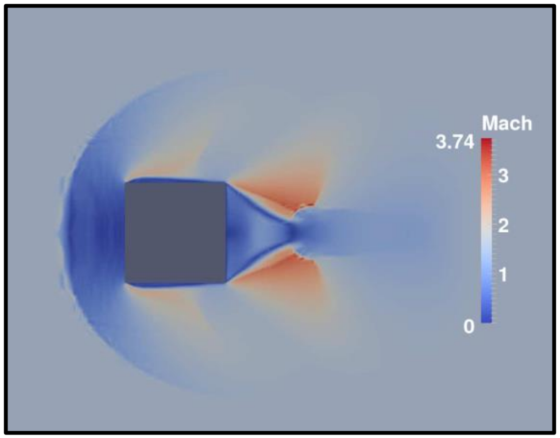
Semi-discrete entropy estimate (1D):

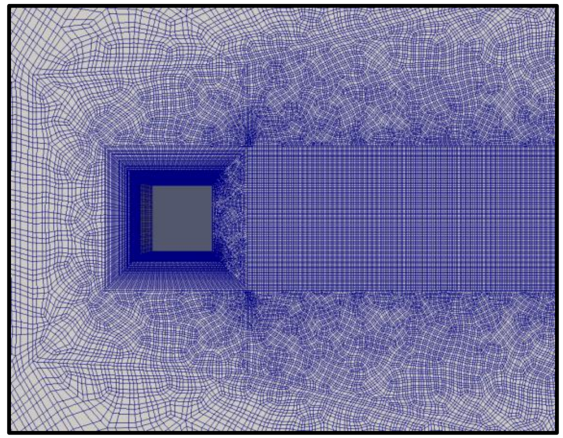
$$\mathbf{1}^\top \mathcal{P} \mathbf{S}_t = \mathbf{w}^\top \mathcal{B}\, \widehat{c}_{11} \mathcal{D} \mathbf{w} - \mathbf{1}^\top \Delta \overline{\mathbf{F}} - (\mathcal{D}\mathbf{w})^\top \mathcal{P}\, \widehat{c}_{11} \,(\mathcal{D}\mathbf{w})$$

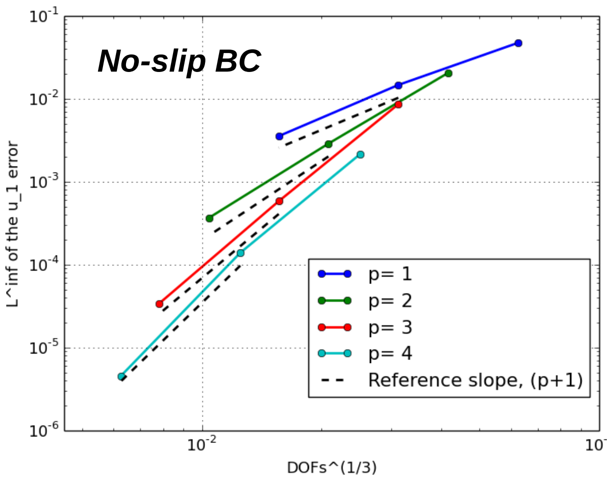
$$\frac{d}{dt} \int_\Omega S \,\mathrm{d}\mathbf{x} = \left[w^\top f_i^{(V)} - F_i\right]_{\partial\Omega} - \int_\Omega w_{x_i}^\top \widehat{c}_{ij}\, w_{x_j} \,\mathrm{d}\mathbf{x}$$

Nonlinearly Stable Wall BCs

Need to design robust, nonlinearly stable wall BCs







$$\mathbf{g}_1^{(B)} = -\underbrace{\left[\overline{\mathbf{f}}_1^{(I)}(\mathbf{q}) - \mathbf{f}_1^{sr}\left(\mathbf{q}, \mathbf{g}^{(E)}\right)\right]}_{\textit{No penetration}} + \underbrace{\left[\overline{\mathbf{f}}_1^{(V)} - \overline{\mathbf{f}}_1^{(V,B)}\right]}_{\textit{Thermal}} + \underbrace{\mathcal{M}\left[\mathbf{w} - \mathbf{g}^{(NS),Vel}\right]}_{\textit{No slip}}$$

Inviscid flux penalty: Flip the sign of the normal velocity component
Viscous flux penalty: Prescribe entropy flow = T_{x1}/T scales with *Re*
Interior penalty: No-slip condition on the velocity; scales with *Re*

Current Status of High-Order FUN3D

Integration with FUN3D

- Implemented as optional library built on low-level FUN3D components
- Leverages much of FUN3D infrastructure, including:
  - GNU Autotools build infrastructure
  - Pre-processing, MPI communication
  - Complex variable, operator overloading functionalities
  - Dynamic overset grid infrastructure, extended to HO elements
  - Regression/performance testing infrastructure
  - Distribution, user training, and user support infrastructure
- FUN3D owns primal grid; library constructs and owns necessary HO data
- Extensive development for compatible domain decomposition
- Conventional FUN3D visualization options available on primal grid; additional I/O options for HO solution
- FUN3D controls overall process flow and routes into HO library as needed, e.g.:
  - *call ssdc_initiate()*
  - *call ssdc_advance_timestep()*
  - *call ssdc_write_soln()*

FUN3D: FEM Basic Features

Temporal Integrators

- Explicit: 4^{th}-Order low-storage RK; feedback controller
- Implicit: BDF(1)(2)(3) and BDF2opt (backward difference formulae)

Solvers

- Nonlinear: (In)Exact Newton-Krylov
  - Trust-region dogleg globalization
- Linear: Right-preconditioned GMRES
  - Exact Jacobian
  - (B)ILU(0), (B)ILU(k), (B)ILUTP (lexicographic)
  - Domain decomposition via additive Schwarz (halo: 1 element)

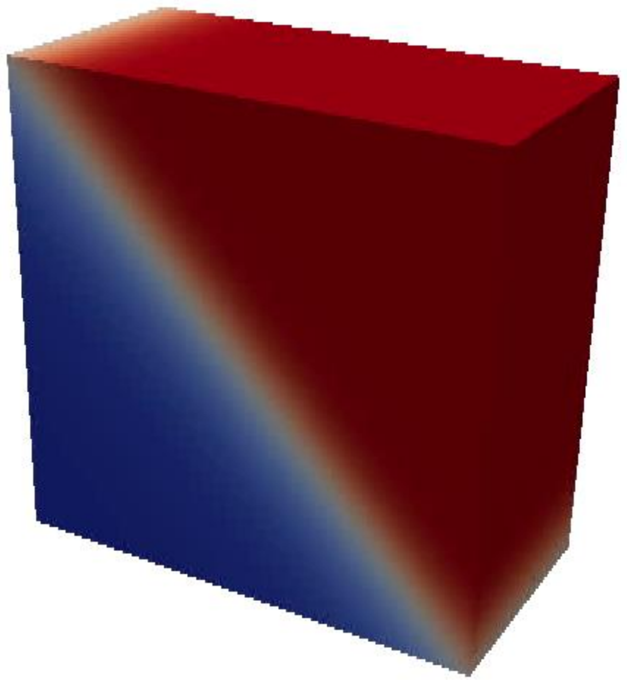
High-Order Definition of Geometry

- Interface with geometry model
- FUN3D elasticity mechanics

Verification and Validation

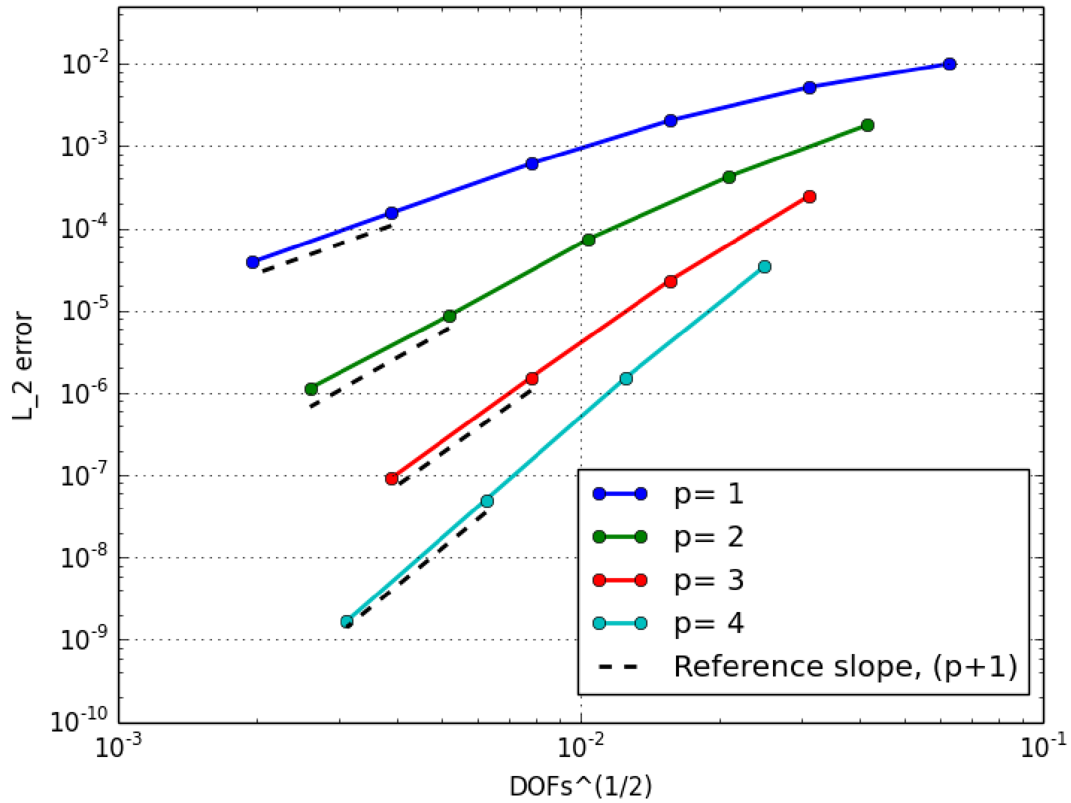
Interior Operator

3D Viscous Shock



Density Field

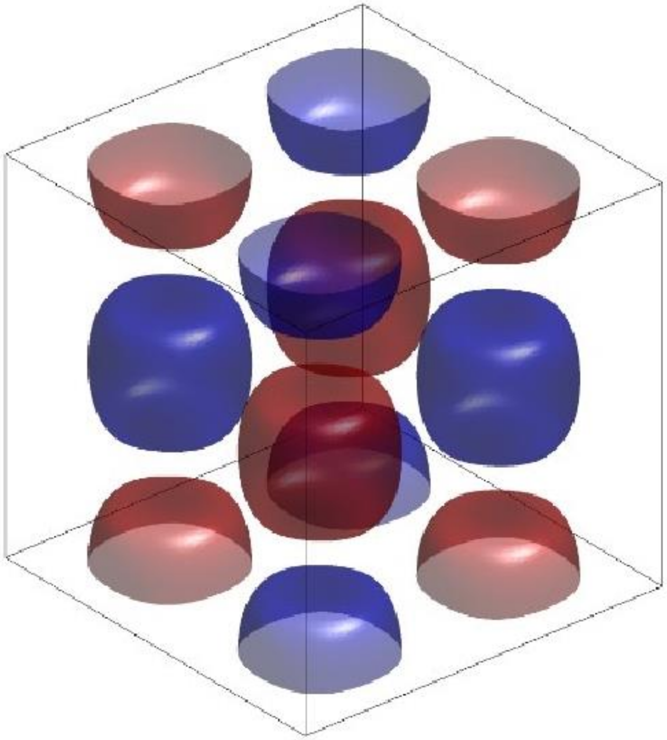
- Exact solution exists for N-S
- Convergence study performed on sequence of nested, highly non-uniform grids



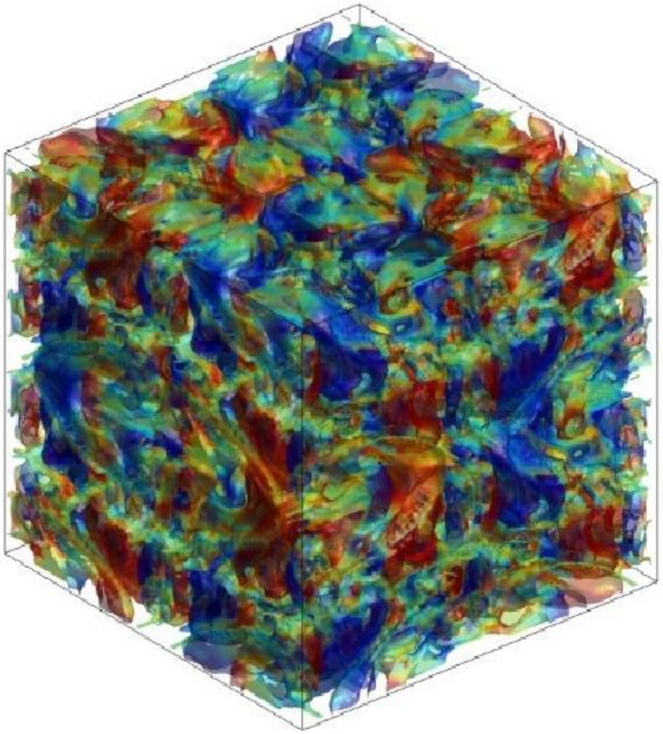
Taylor-Green Vortex

Re=1600, M_∞=0.1

Iso-surface of the z-component of vorticity



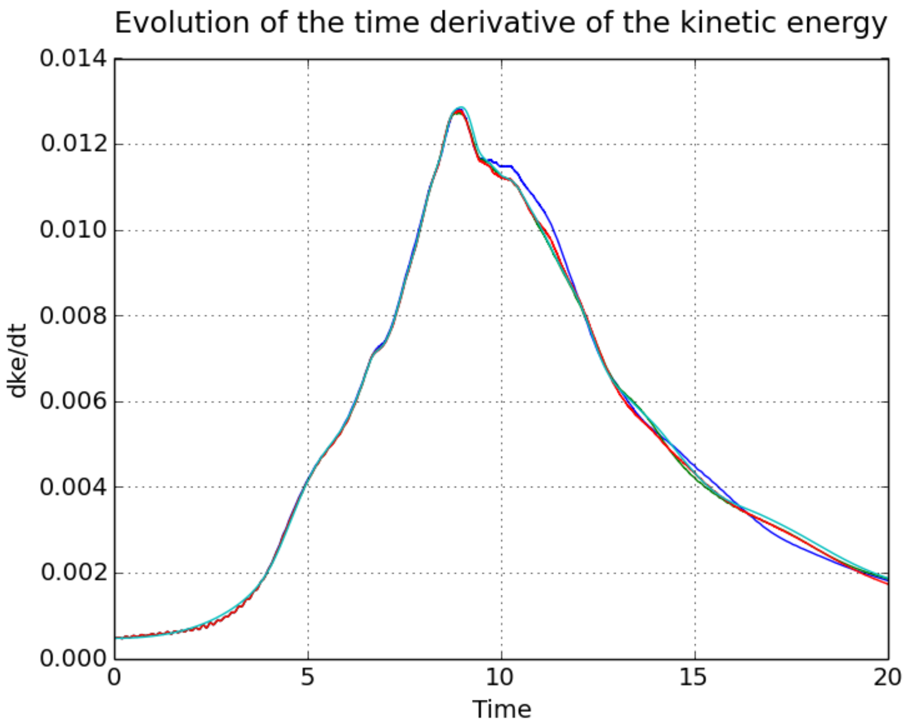
t = 0

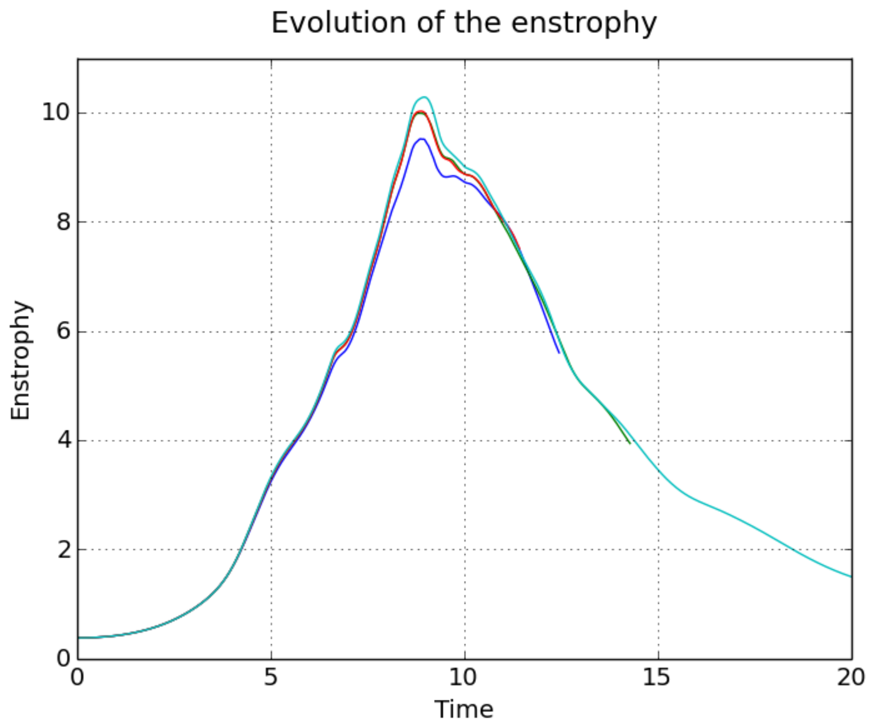


t = 20

Taylor-Green Vortex

Evolution of Kinetic Energy and Enstrophy





p = 2 with 128^3 elements

p = 3 with 96^3 elements

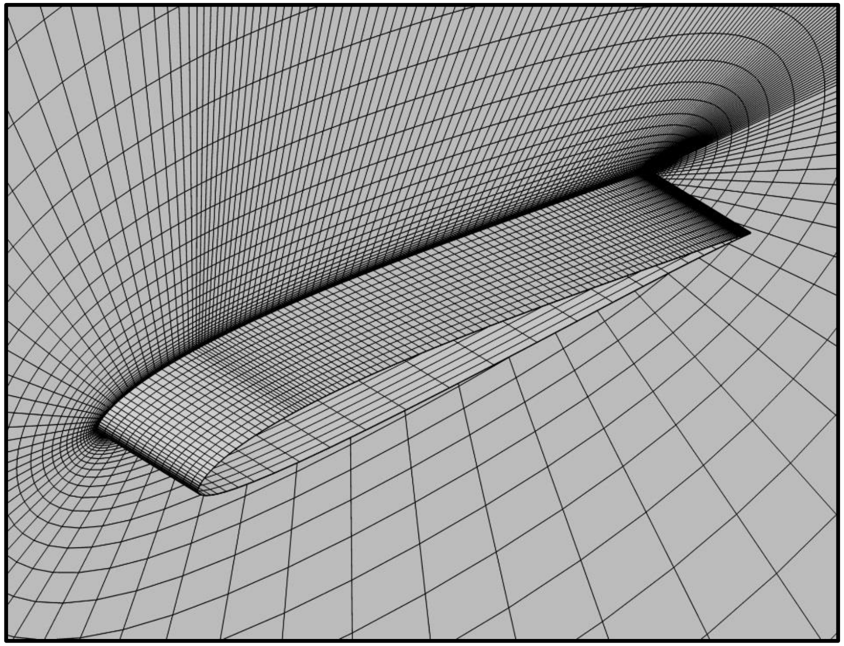
p = 4 with 64^3 elements

Hillewaert et al; spectral method with 512^3 elements

SD7003 Airfoil Test Case

Background

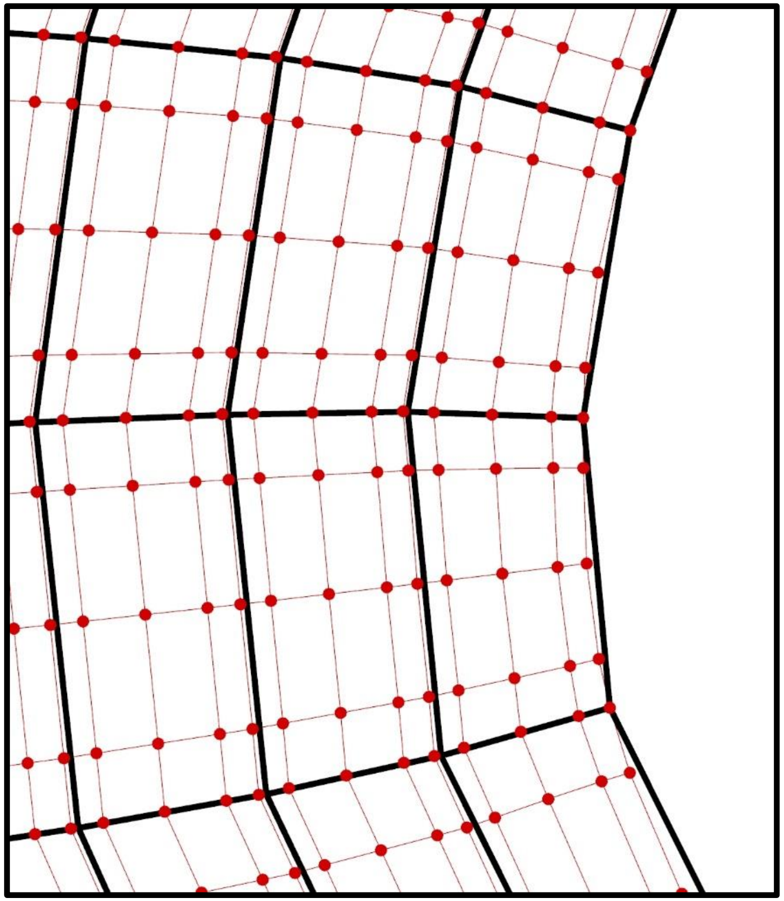
- Standard benchmark test case for 2nd high-order workshop (C3.3, “difficult”)
- $M_\infty = 0.1$, $\alpha = 8^\circ$, $Re_c = 60{,}000$
- Should show small region of laminar separation on upper surface followed by transition to turbulent flow downstream
- Grid is 179 x 55 x 15: 134,568 hexes with periodic sidewalls
- BDF2opt run from freestream to approximately 8 convection times
- FUN3D solutions shown are isosurfaces of velocity magnitude colored by pressure

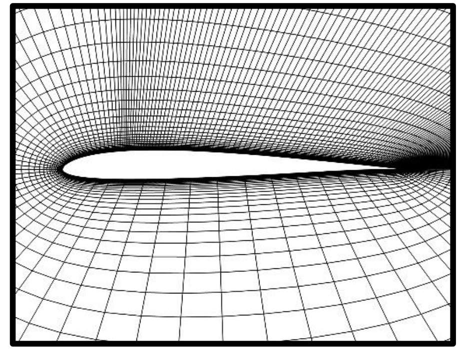


SD7003 Test Case

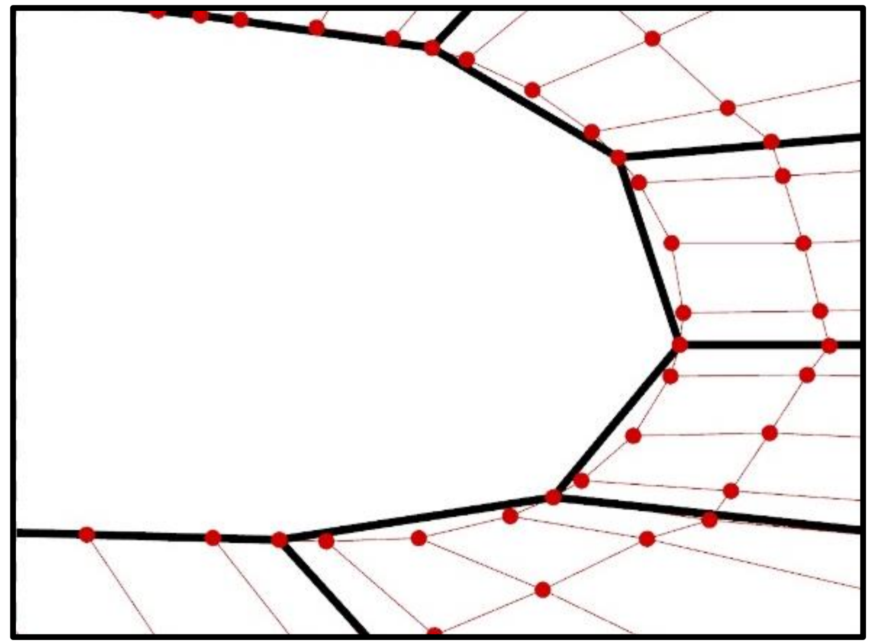
Geometry Considerations

Leading Edge





Trailing Edge



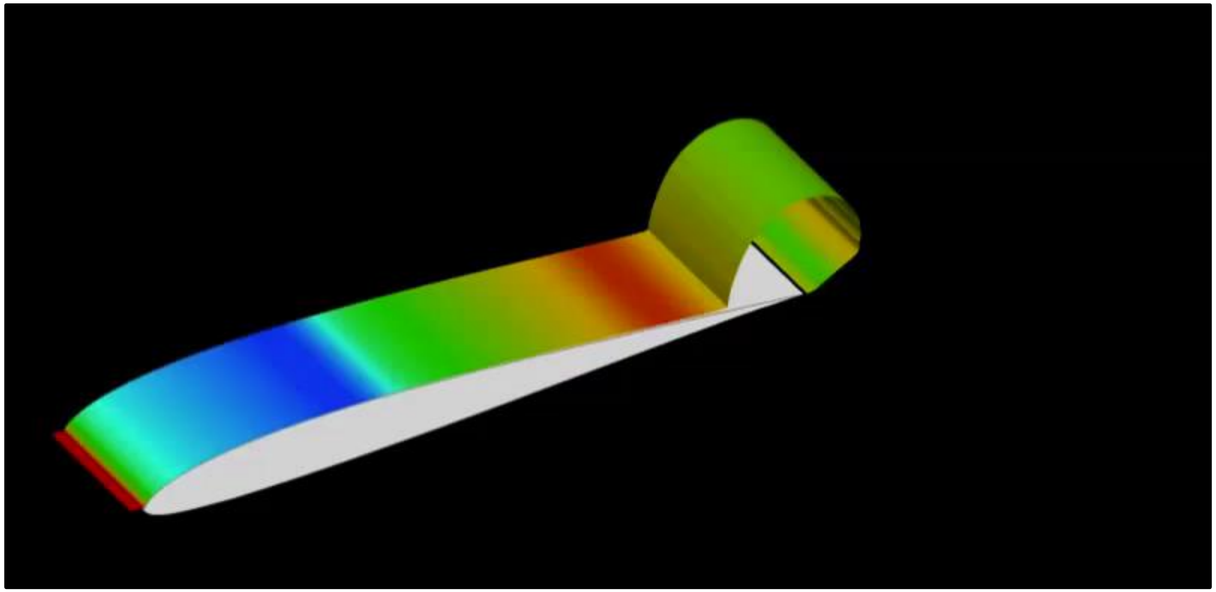
- p = 4 solution points shown: surface points are projected to the geometry
- Mesh interior is deformed using existing FUN3D linear elasticity mechanics

SD7003 Test Case

Finite Volume Scheme vs Entropy-Stable Scheme with p = 1

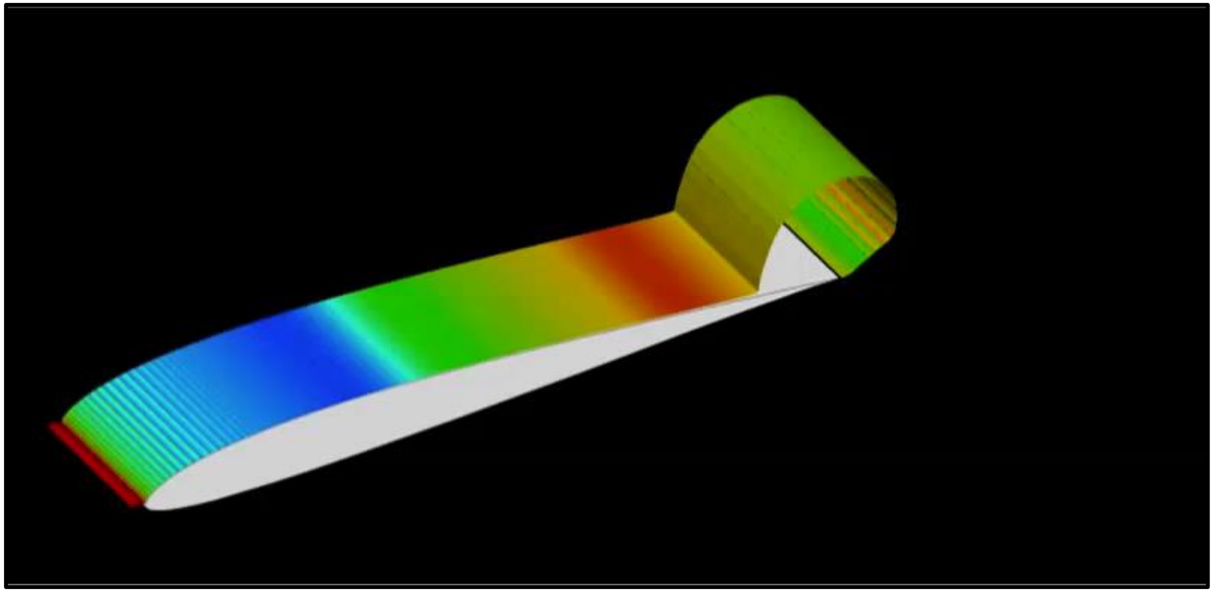
Standard FUN3D Second-Order Finite Volume Scheme

- 147,675 DOFs
- Shows mild spanwise variations very late



Entropy-Stable Scheme with p = 1 (second order)

- 134,568 DOFs
- Does not develop spanwise variations
- Discontinuities at element interfaces clearly visible

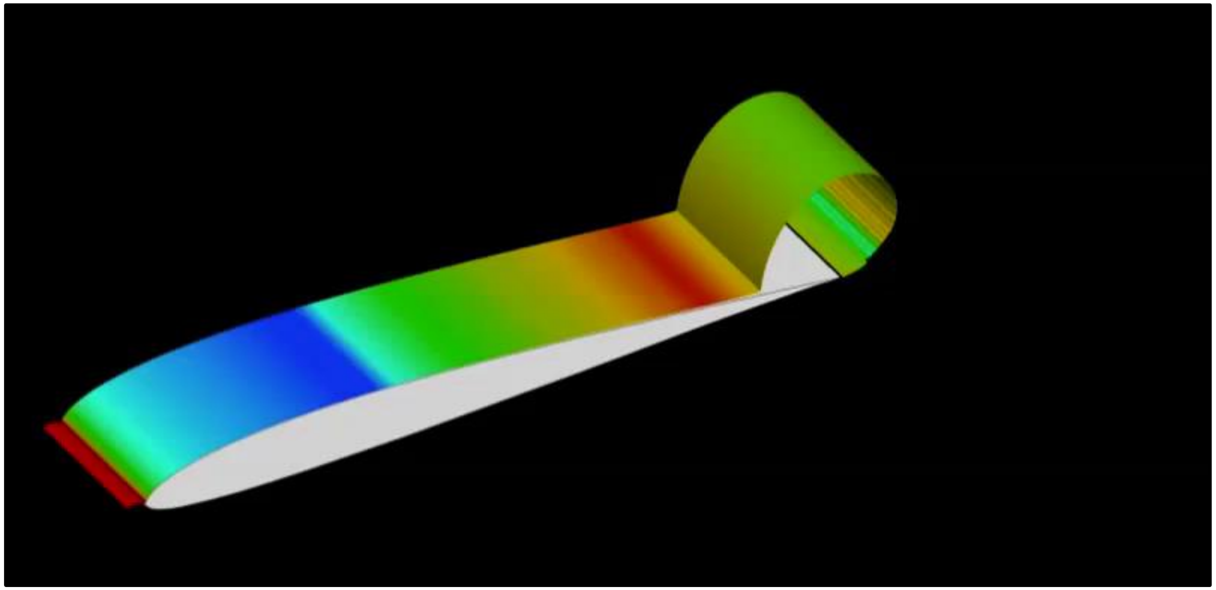


SD7003 Test Case

Entropy-Stable Scheme with p = 2, 3

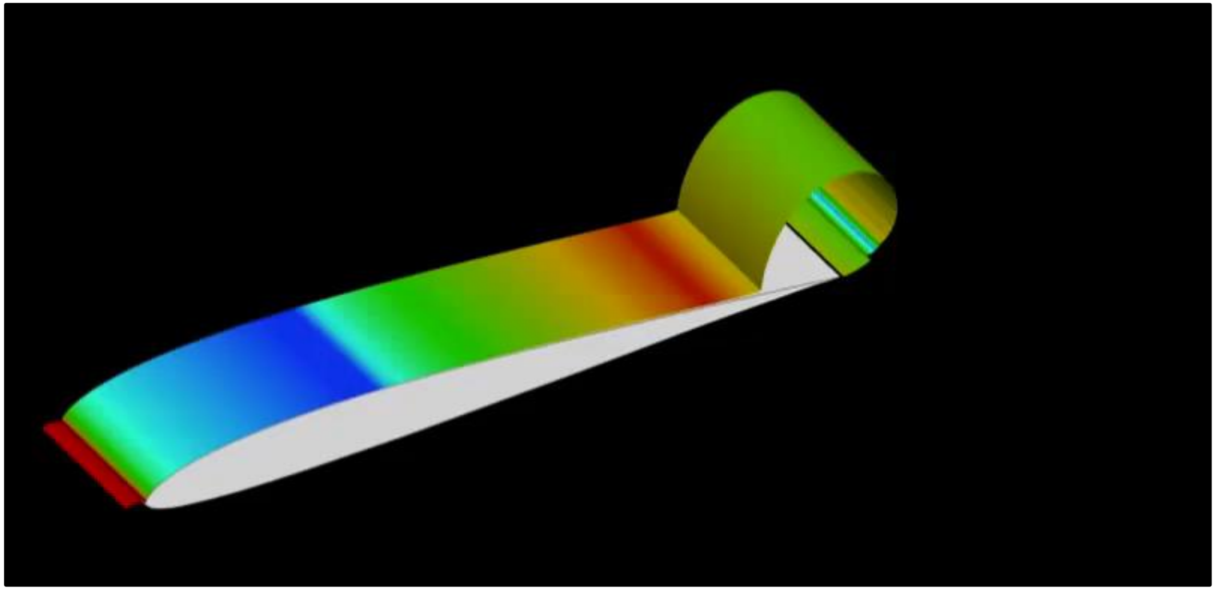
Entropy-Stable Scheme with p = 2 (third order)

- 3,633,336 DOFs
- Shows spanwise breakdown and develops expected behavior



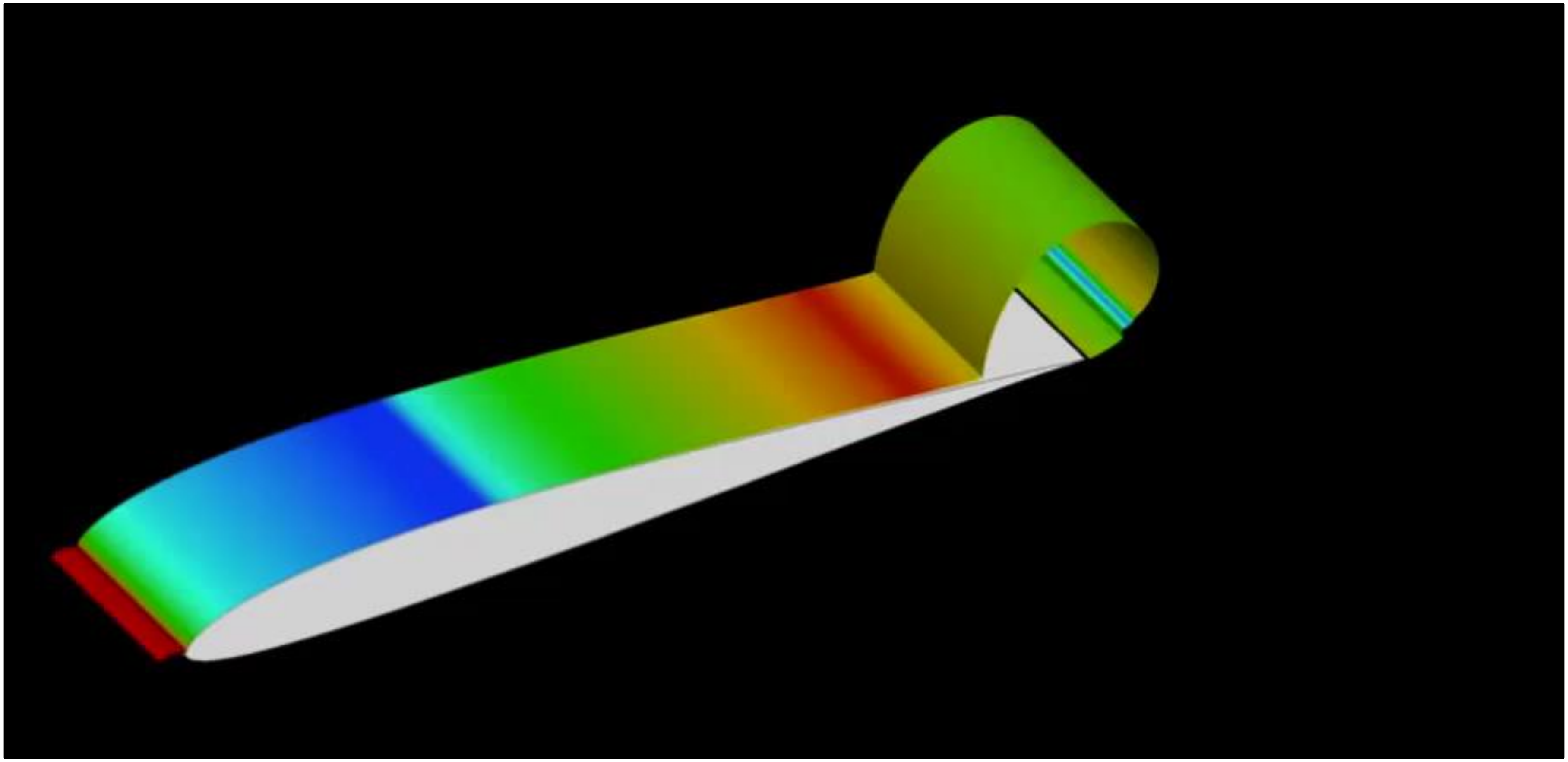
Entropy-Stable Scheme with p = 3 (fourth order)

- 8,612,352 DOFs
- Fine-scale features start to appear, transition shifts downstream



SD7003 Test Case

Entropy-Stable Scheme with p = 4

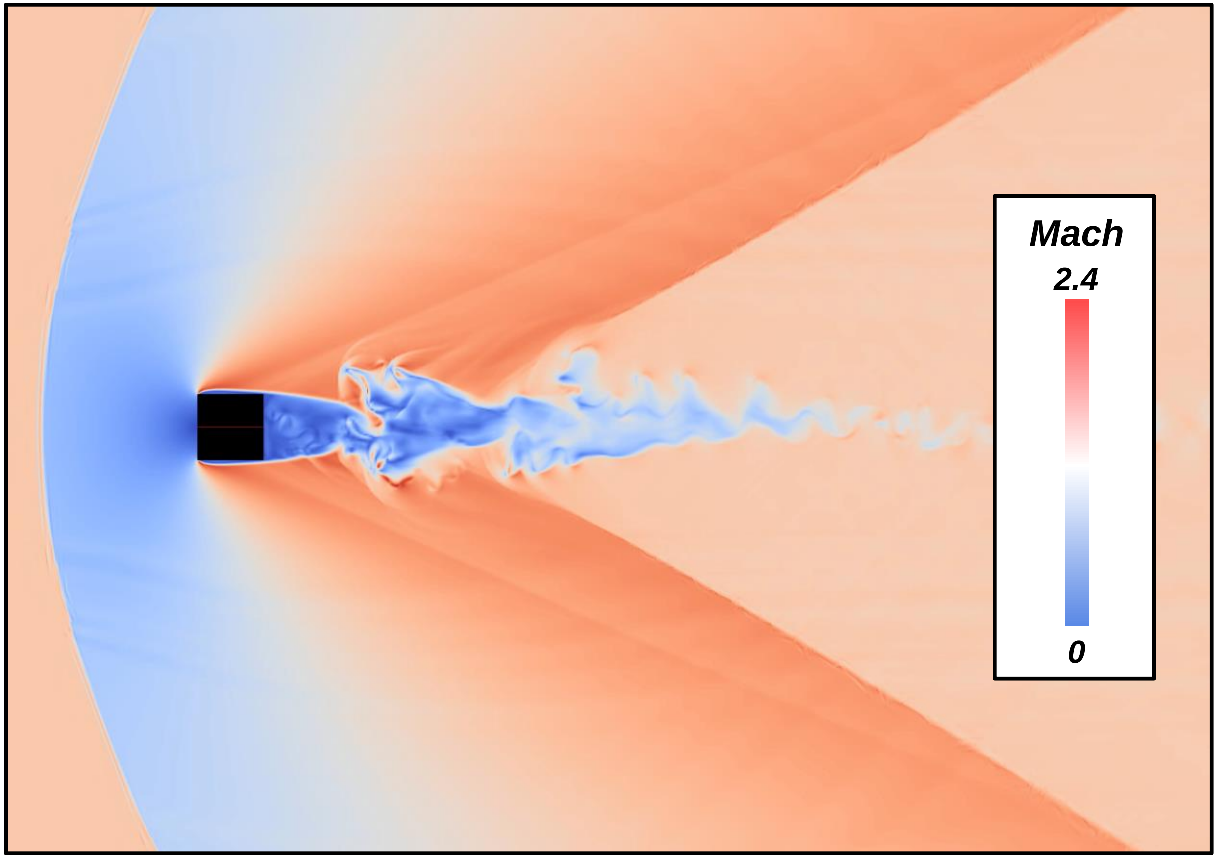


Entropy-Stable Scheme with p = 4 (fifth order)

- 16,821,000 DOFs
- Good qualitative resolution of expected flow physics

Supersonic Flow Past 3D Square Cylinder

Re = 10,000 $M_\infty = 1.5$ p = 3 (fourth order)



- 2,048,000 DOFs
- No dealiasing, artificial dissipation, or filtering

Conclusions

Raising the bar on high-order CFD:
Building a firm mathematical foundation for nonlinear stability

- If the code blows up, there's a bug
- Entropy conservation and stability using DG-FEM SBP operator
- First known nonlinearly stable no-slip wall BCs at any order
- All test cases demonstrate design order accuracy for smooth flows
- Noteworthy robustness for shocks even without additional dissipation or limiting

Foundational Algorithmic Development

- Entropy stability of all boundary conditions
- Entropy stability of turbulence equations including source terms
- Entropy stability for all schemes on all element types
- Provable stability of nonlinear iteration operator
- Prove stability of regularized reverse time adjoint operator
- DONE: August 18, 2019

Backup Material

Stability of High-Order Schemes:

Compressible Navier-Stokes Equations

Mathematical entropy (Continuous → Discrete)

- Convex extension of original equations (Friedrichs / Lax)
- Formed by contracting N-S equations with entropy variables
- Bounded physical quantity (N-S equations → thermodynamic entropy)

What does it buy you?

- Nonlinear stability in L^2
  - Entropy is bounded from above in an integral sense
  - The code doesn't "blow up" (well, usually…see below)
- The nonlinear stability plateau for N-S equations

What it doesn't guarantee

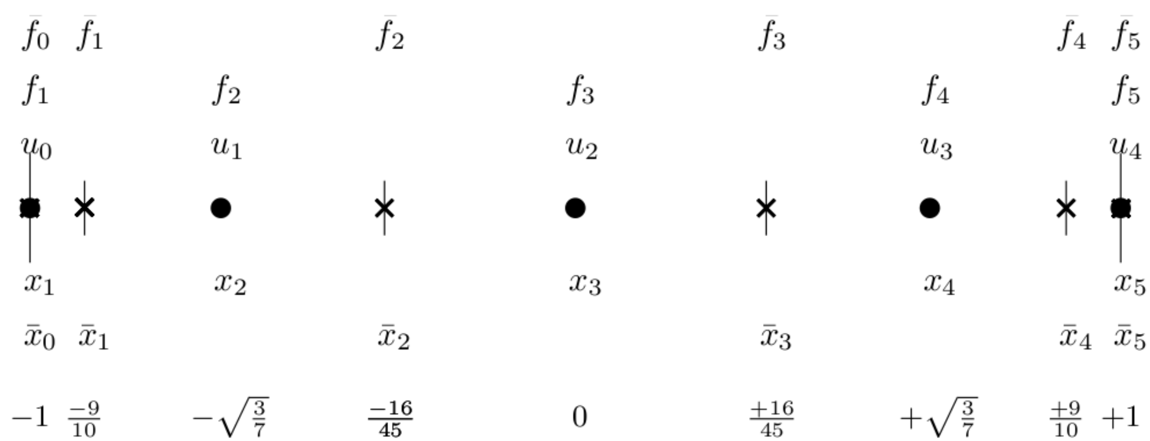
- Positivity (e.g., negative temperatures)
  - Shu's limiter (RCA NRA with Brown Univ)

Telescopic Flux Form

$$f_x(\mathbf{q}) = \mathcal{D}\mathbf{f} + \mathcal{T}_{p+1} = \mathcal{P}^{-1}\Delta\bar{\mathbf{f}} + \mathcal{T}_{p+1}, \quad \mathcal{T}_{p+1} = \text{trunc. error}$$

$$\Delta = \begin{pmatrix} -1 & 1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 & 0 \\ 0 & 0 & \ddots & \ddots & 0 & 0 \\ 0 & 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 1 \end{pmatrix} \rightarrow [N \times (N+1)]$$

Δ: calculates undivided difference of adjacent fluxes



A Quick Review of Stability Proofs

Linear advection equation

$$u\left[\frac{\partial u}{\partial t}+a\frac{\partial u}{\partial x}=0\right]; \quad \int_{-1}^{+1}\left(\frac{\partial \frac{u^2}{2}}{\partial t}+a\frac{\partial \frac{u^2}{2}}{\partial x}=0\right); \quad \frac{1}{2}\frac{\partial}{\partial t}||u||^2=\left(-a\frac{u^2}{2}\right)\Big]_{-1}^{+1}$$

Burgers' equation

$$u\left[\frac{\partial u}{\partial t}+\frac{1}{2}\frac{\partial u^2}{\partial x}=\epsilon\frac{\partial^2 u}{\partial x^2}\right] \quad ; \quad \frac{1}{2}\frac{\partial}{\partial t}||u||^2+\epsilon||\frac{\partial u}{\partial x}||^2=\left(\epsilon\frac{\partial \frac{u^2}{2}}{\partial x}-\frac{2u}{3}\frac{u^2}{2}\right)\Big]_{-1}^{+1}$$

Incompressible Navier-Stokes equations

$$u_i\left[\rho\frac{\partial u_i}{\partial t}+\rho\frac{\partial u_j u_i}{\partial x_j}+\frac{\partial p\delta_{ij}}{\partial x_j}=\frac{\partial}{\partial x_j}\epsilon\frac{\partial u_i}{\partial x_j} \quad ; \quad \frac{\partial u_i}{\partial x_i}=0\right] \quad ;$$

$$\rho\frac{\partial}{\partial t}||\frac{1}{2}u_k u_k||^2+\epsilon||\frac{\partial u_i}{\partial x_j}||^2=\left(\epsilon\frac{\partial \frac{1}{2}u_k u_k}{\partial x_j}-u_j(\frac{1}{2}u_k u_k+p)\delta_{ij}\right)\Big]_{\partial S} \quad ;$$

Compressible Navier-Stokes?

Summation-by-Parts Operators

Integration by parts:

$$\int_{x_L}^{x_R} \phi q_x \,\mathrm{d}x = \phi q|_{x_L}^{x_R} - \int_{x_L}^{x_R} \phi_x q \,\mathrm{d}x$$

Semi-discrete:

$$\boldsymbol{\phi}^\top \mathcal{P}\mathcal{P}^{-1}\mathcal{Q}\mathbf{q} = \boldsymbol{\phi}^\top \left(\mathcal{B} - \mathcal{Q}^\top\right)\mathbf{q} = \phi_N q_N - \phi_1 q_1 - \boldsymbol{\phi}^\top \mathcal{D}^\top \mathcal{P}\mathbf{q}$$

Mimetic form for first derivative $\mathcal{D}\boldsymbol{\phi}$ if:

$$\mathcal{D} = \mathcal{P}^{-1}\mathcal{Q}, \quad \mathcal{P} = \mathcal{P}^\top, \quad \zeta^\top \mathcal{P}\zeta > 0, \quad \zeta \neq \mathbf{0},$$
$$\mathcal{Q}^\top = \mathcal{B} - \mathcal{Q}, \quad \mathcal{B} = \mathrm{diag}\left(-1, 0, \ldots, 0, 1\right)$$

Nonlinearly Stable Wall BCs

- 3-D square cylinder with nonuniform grid
- Re = 200, M = 0.1
- Scheme retains accuracy on boundary